



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2022 – 02:11 PM EDT

PDB ID : 7N6H  
Title : The crystal structure of the GH30 subfamily 10 enzyme, AcXbh30A from *Acetivibrio clariflavus*  
Authors : Tan, K.; St John, F.J.  
Deposited on : 2021-06-08  
Resolution : 1.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

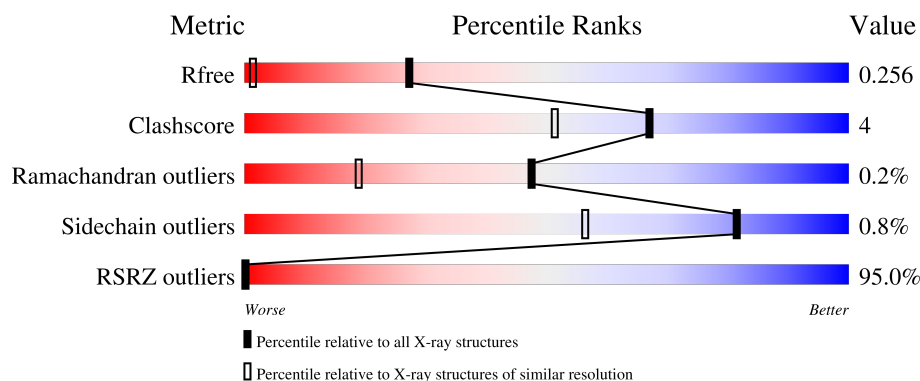
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1850 (1.30-1.26)
Clashscore	141614	1926 (1.30-1.26)
Ramachandran outliers	138981	1860 (1.30-1.26)
Sidechain outliers	138945	1859 (1.30-1.26)
RSRZ outliers	127900	1807 (1.30-1.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	<div> <div>92%</div> <div>89% 9%</div> </div>
1	B	444	<div> <div>93%</div> <div>88% 9%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	504	-	-	-	X
2	CL	A	506	-	-	-	X
2	CL	A	508	-	-	X	-
2	CL	A	511	-	-	-	X
2	CL	A	515	-	-	X	-
2	CL	B	503	-	-	X	-
2	CL	B	507	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AcXbh30A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3454	2194	570	679	11			
1	B	433	Total	C	N	O	S	0	1	0
			3443	2187	569	676	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP G8LU16
A	464	LEU	-	expression tag	UNP G8LU16
A	465	GLU	-	expression tag	UNP G8LU16
A	466	HIS	-	expression tag	UNP G8LU16
A	467	HIS	-	expression tag	UNP G8LU16
A	468	HIS	-	expression tag	UNP G8LU16
A	469	HIS	-	expression tag	UNP G8LU16
A	470	HIS	-	expression tag	UNP G8LU16
A	471	HIS	-	expression tag	UNP G8LU16
B	28	MET	-	initiating methionine	UNP G8LU16
B	464	LEU	-	expression tag	UNP G8LU16
B	465	GLU	-	expression tag	UNP G8LU16
B	466	HIS	-	expression tag	UNP G8LU16
B	467	HIS	-	expression tag	UNP G8LU16
B	468	HIS	-	expression tag	UNP G8LU16
B	469	HIS	-	expression tag	UNP G8LU16
B	470	HIS	-	expression tag	UNP G8LU16
B	471	HIS	-	expression tag	UNP G8LU16

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	Cl	0	0
			15	15		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Cl	0	0
			8	8		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	388	Total	O	0	0
			388	388		
4	B	329	Total	O	0	0
			329	329		

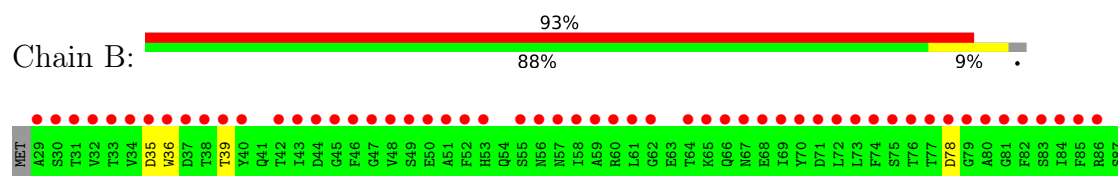
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: AcXbh30A



#### • Molecule 1: AcXbh30A



A448	P388	C328	G268	S208	M148	I88
P449	K389	F329	S269	P209	M149	L89
M450	T390	K330	S270	E210	K150	G90
S451	G391	T331	Y271	E211	T151	D91
I452	K392	N332	I272	L212	N152	G92
T453	F393	N333	P273	R213	G153	G93
T454	A394	G334	F274	I214	S154	T94
F455	I395	E335	T275	F215	V155	M95
V396	V396	G336	T276	M216	V156	G96
O457	A397	L337	T277	M217	G157	M97
D458	I398	I338	K278	D218	A98	A98
T459	N399	K339	S279	Y219	D99	D99
E460	M400	K340	K280	L220	D100	D100
S461	G401	D341	G281	V221	G101	G101
ALA	W402	L342	G282	T222	P102	P102
SER	S403	N343	G283	T223	M103	M103
LEU	K404	S344	I284	F224	K104	K104
GLU	Q405	K345	W285	D225	T105	T105
HIS	S406	T346	M286	K226	M106	M106
HIS	I407	Y347	T287	E227	Q107	Q107
HIS	T408	K348	E288	M228	P108	P108
HIS	Y409	V349	V289	I229	A109	A109
HIS	T410	A350	S290	T230	E110	E110
HIS	L411	K351	D291	A231	D111	D111
	K412	R352	M292	K232	V112	V112
	G413	L353	N293	V233	W113	W113
	F414	Y354	G294	F234	D114	D114
	S415	T355	N295	F235	W115	W115
	P416	I356	D296	A236	M116	M116
	A417	G357	T297	E237	E117	E117
	S418	Q358	T298	M238	S118	S118
	V419	F359	I299	N239	M119	M119
	T420	S360	N300	S240	D120	D120
	P421	R361	D301	F241	S121	S121
	Y422	F362	G302	N242	Q122	Q122
	T423	I363	L303	E243	I123	I123
	T424	R364	R304	Q244	P124	P124
	S425	P365	W305	Y245	M125	M125
	S426	G366	A306	A246	I126	I126
	T427	W367	K307	I247	M127	M127
	Q428	Q368	E308	N248	A128	A128
	M429	R369	I309	S249	I129	I129
	L430	I370	H310	L250	Q130	Q130
	E431	E371	D311	N251	S131	S131
	K432	A372	F312	D252	K132	K132
	G433	T373	M313	P253	Y133	Y133
	S434	K374	T314	L254	G134	G134
	D435	N375	I315	A255	V135	V135
	I436	P376	T316	V256	D136	D136
	T437	W377	F317	K257	Q137	Q137
	V438	S378	G318	R258	I138	I138
	M439	N379	N319	V259	L139	L139
	M440	V380	A320	D260	Y140	Y140
	S441	Y381	W321	L261	S201	S201
	S442	V382	F322	V262	Y202	Y202
	F443	T383	Y323	Q263	W143	W143
	S444	A384	W324	A264	S144	S144
	F445	Y385	W325	H265	P145	P145
	E446	K386	G326	M266	R206	R206
	L447	D387	A327	Y267	W207	W207

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.87Å 108.02Å 66.84Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	41.18 – 1.28 41.18 – 1.28	Depositor EDS
% Data completeness (in resolution range)	96.3 (41.18-1.28) 96.2 (41.18-1.28)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	13.51 (at 1.28Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, $R_{free}$	0.202 , 0.254 0.203 , 0.256	Depositor DCC
$R_{free}$ test set	10529 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 26.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.387 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.24	0/3544	0.47	0/4821
1	B	0.24	0/3533	0.46	0/4806
All	All	0.24	0/7077	0.47	0/9627

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3454	0	3292	24	0
1	B	3443	0	3281	24	0
2	A	15	0	0	8	0
2	B	8	0	0	5	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
4	A	388	0	0	4	0
4	B	329	0	0	3	0
All	All	7649	0	6582	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:510:CL:CL	4:A:896:HOH:O	2.38	0.78
1:A:213:ARG:NE	2:A:503:CL:CL	2.50	0.73
2:A:515:CL:CL	4:A:860:HOH:O	2.43	0.73
2:A:514:CL:CL	4:A:952:HOH:O	2.53	0.61
1:A:404:LYS:HG3	1:A:449:PRO:HD3	1.85	0.59
1:A:196:PRO:HG3	1:A:236:ALA:HB1	1.86	0.58
1:B:196:PRO:HG3	1:B:236:ALA:HB1	1.88	0.56
1:A:399:ASN:ND2	2:A:515:CL:CL	2.69	0.56
1:B:123:ILE:HG23	1:B:185:ILE:HD11	1.91	0.53
1:A:48:VAL:HG12	1:A:323:TYR:HB3	1.91	0.53
1:B:217:ARG:HA	4:B:728:HOH:O	2.09	0.53
1:A:171:TYR:O	1:A:175:HIS:ND1	2.39	0.52
1:B:98:ALA:N	2:B:508:CL:CL	2.80	0.52
2:B:503:CL:CL	4:B:902:HOH:O	2.56	0.51
1:A:36:TRP:HB2	1:A:414:PHE:CD1	2.46	0.51
1:B:36:TRP:HB2	1:B:414:PHE:CD1	2.46	0.51
1:A:249:SER:OG	2:A:508:CL:CL	2.61	0.51
1:B:290:SER:HB2	1:B:335:GLU:HA	1.94	0.49
1:B:252:ASP:HB3	1:B:255:ALA:HB3	1.95	0.49
1:A:290:SER:HB2	1:A:335:GLU:HA	1.94	0.48
1:A:123:ILE:HG23	1:A:185:ILE:HD11	1.95	0.48
1:B:104:LYS:HG2	2:B:505:CL:CL	2.52	0.46
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.68	0.46
1:B:374:LYS:HE2	1:B:374:LYS:HB2	1.81	0.46
1:A:40:TYR:OH	1:A:371:GLU:OE2	2.34	0.46
1:A:130:GLN:HG2	1:A:135:VAL:O	2.16	0.45
1:B:312:PHE:CZ	1:B:318:GLY:HA3	2.51	0.45
1:B:206:ARG:O	2:B:507:CL:CL	2.72	0.45
1:B:149:MET:HE1	1:B:171:TYR:HB2	1.99	0.45
1:A:248:ASN:HB2	2:A:508:CL:CL	2.54	0.45
1:A:243:GLU:O	1:A:247:ILE:HG13	2.17	0.44
1:A:312:PHE:CZ	1:A:318:GLY:HA3	2.52	0.44
1:A:271:TYR:OH	1:A:308:GLU:OE1	2.22	0.44
1:A:377:VAL:HG22	1:A:378:SER:H	1.83	0.44
1:A:412:LYS:NZ	4:A:628:HOH:O	2.49	0.44
1:B:243:GLU:O	1:B:247:ILE:HG13	2.17	0.43
1:A:249:SER:N	2:A:508:CL:CL	2.89	0.43
1:B:39:THR:HG22	1:B:370:ILE:HG22	2.00	0.43
1:B:171:TYR:O	1:B:175:HIS:ND1	2.49	0.43
1:A:107:GLN:HB2	1:A:113:TRP:CZ3	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ASP:HB3	1:B:371:GLU:HB3	2.00	0.42
2:B:503:CL:CL	4:B:642:HOH:O	2.59	0.42
1:B:78:ASP:N	1:B:78:ASP:OD1	2.51	0.41
1:A:196:PRO:HB2	1:A:207:TRP:HB2	2.01	0.41
1:B:130:GLN:HG2	1:B:135:VAL:O	2.19	0.41
1:B:168:TYR:OH	1:B:192:ILE:O	2.31	0.41
1:B:193:GLN:HG2	1:B:207:TRP:CD1	2.56	0.41
1:B:377:VAL:HG22	1:B:378:SER:H	1.85	0.41
1:A:193:GLN:HG2	1:A:207:TRP:CD1	2.56	0.41
1:B:380:VAL:HA	1:B:398:ILE:O	2.21	0.41
1:B:110:GLU:HB3	1:B:148:TRP:CZ3	2.56	0.40
1:A:404:LYS:H	1:A:404:LYS:HD2	1.84	0.40
1:B:261:ILE:HD13	1:B:285:TRP:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/444 (98%)	418 (96%)	14 (3%)	1 (0%)	47	19
1	B	432/444 (97%)	418 (97%)	13 (3%)	1 (0%)	47	19
All	All	865/888 (97%)	836 (97%)	27 (3%)	2 (0%)	47	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	TRP
1	B	324	TRP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/384 (98%)	373 (99%)	3 (1%)	81	56
1	B	374/384 (97%)	371 (99%)	3 (1%)	81	56
All	All	750/768 (98%)	744 (99%)	6 (1%)	81	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	324	TRP
1	A	329	PHE
1	B	324	TRP
1	B	329	PHE
1	B	378	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 23 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	A	517	-	3,3,3	1.25	0	3,3,3	1.32	0
3	ACT	B	509	-	3,3,3	1.28	0	3,3,3	1.27	0
3	ACT	A	516	-	3,3,3	1.27	0	3,3,3	1.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	433/444 (97%)	4.62	410 (94%) <b>0</b> <b>0</b>	10, 15, 21, 38	0
1	B	433/444 (97%)	4.76	413 (95%) <b>0</b> <b>0</b>	9, 14, 21, 34	0
All	All	866/888 (97%)	4.69	823 (95%) <b>0</b> <b>0</b>	9, 15, 21, 38	0

All (823) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ALA	36.8
1	B	306	ALA	14.5
1	B	146	PRO	12.5
1	B	246	ALA	11.7
1	B	329	PHE	11.5
1	A	338	ILE	11.2
1	B	402	TRP	11.2
1	A	293	ASN	11.0
1	A	135	VAL	11.0
1	B	219	TYR	10.7
1	B	456	VAL	10.5
1	A	359	PHE	10.5
1	B	108	PRO	10.4
1	A	279	SER	10.4
1	B	190	ILE	10.2
1	B	82	PHE	10.1
1	A	315	ILE	10.0
1	A	198	LEU	9.9
1	B	417	ALA	9.7
1	B	347	TYR	9.7
1	B	299	ILE	9.7
1	A	241	PHE	9.6
1	A	33	THR	9.6
1	B	430	LEU	9.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	247	ILE	9.5
1	B	156	VAL	9.5
1	B	411	LEU	9.5
1	A	259	VAL	9.5
1	A	324	TRP	9.5
1	A	247	ILE	9.4
1	B	370	ILE	9.4
1	B	327	ALA	9.4
1	B	52	PHE	9.3
1	B	285	TRP	9.3
1	B	84	ILE	9.3
1	B	284	ILE	9.3
1	A	207	TRP	9.2
1	A	168	TYR	9.2
1	B	112	VAL	9.1
1	B	187	ILE	9.0
1	B	409	TYR	9.0
1	A	129	ILE	8.9
1	B	70	TYR	8.8
1	A	274	PHE	8.8
1	B	427	THR	8.7
1	A	40	TYR	8.7
1	A	74	PHE	8.7
1	B	38	THR	8.7
1	A	48	VAL	8.6
1	A	32	VAL	8.6
1	B	188	THR	8.5
1	A	138	ILE	8.5
1	B	212	LEU	8.4
1	B	223	THR	8.4
1	A	299	ILE	8.4
1	A	133	TYR	8.3
1	A	43	ILE	8.3
1	B	303	LEU	8.2
1	B	148	TRP	8.2
1	A	123	ILE	8.2
1	B	381	TYR	8.2
1	A	221	VAL	8.2
1	A	271	TYR	8.2
1	A	105	THR	8.2
1	A	155	VAL	8.1
1	A	367	TRP	8.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	254	ILE	8.1
1	A	419	VAL	8.1
1	A	46	PHE	8.1
1	A	215	PHE	8.1
1	B	179	TYR	8.1
1	B	89	LEU	8.0
1	B	389	LYS	8.0
1	B	123	ILE	8.0
1	A	250	LEU	8.0
1	A	172	LEU	7.9
1	B	309	ILE	7.8
1	B	46	PHE	7.8
1	A	439	ASN	7.8
1	B	233	VAL	7.8
1	A	170	THR	7.7
1	B	31	THR	7.7
1	B	445	PHE	7.7
1	B	271	TYR	7.7
1	B	207	TRP	7.6
1	A	303	LEU	7.6
1	B	151	THR	7.6
1	A	321	TRP	7.6
1	A	224	PHE	7.6
1	A	145	PRO	7.6
1	A	455	PHE	7.5
1	B	274	PHE	7.5
1	A	402	TRP	7.5
1	A	456[A]	VAL	7.5
1	B	261	ILE	7.4
1	B	443	PHE	7.4
1	B	165	TYR	7.4
1	A	222	PRO	7.4
1	A	160	LEU	7.4
1	A	390	THR	7.4
1	B	133	TYR	7.4
1	B	202	TYR	7.3
1	A	331	THR	7.3
1	A	452	ILE	7.3
1	B	43	ILE	7.3
1	A	118	SER	7.2
1	B	270	SER	7.2
1	A	461	SER	7.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	7.2
1	A	309	ILE	7.1
1	B	436	ILE	7.1
1	A	61	LEU	7.1
1	A	285	TRP	7.1
1	A	142	VAL	7.1
1	A	64	THR	7.1
1	A	261	ILE	7.1
1	B	116	ASN	7.1
1	A	393	PHE	7.1
1	A	408	THR	7.1
1	B	290	SER	7.0
1	A	231	ALA	7.0
1	B	235	PHE	7.0
1	B	414	PHE	7.0
1	A	412	LYS	7.0
1	A	329	PHE	7.0
1	A	31	THR	7.0
1	A	176	ILE	6.9
1	A	113	TRP	6.9
1	B	115	TRP	6.9
1	B	437	THR	6.9
1	A	29	ALA	6.9
1	A	430	LEU	6.9
1	B	424	THR	6.8
1	B	109	ALA	6.8
1	A	438	VAL	6.8
1	B	143	TRP	6.8
1	A	391	GLY	6.8
1	B	214	ILE	6.8
1	A	305	TRP	6.8
1	B	59	ALA	6.8
1	A	92	GLY	6.7
1	A	69	ILE	6.7
1	A	354	TYR	6.7
1	B	367	TRP	6.7
1	A	66	GLN	6.6
1	A	89	LEU	6.6
1	B	236	ALA	6.6
1	A	34	VAL	6.6
1	B	362	PHE	6.6
1	A	30	SER	6.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	441	SER	6.5
1	A	394	ALA	6.5
1	A	322	PHE	6.5
1	A	76	THR	6.5
1	A	229	ILE	6.5
1	A	459	THR	6.5
1	B	51	ALA	6.5
1	A	414	PHE	6.5
1	B	230	THR	6.5
1	A	185	ILE	6.5
1	B	415	SER	6.5
1	B	452	ILE	6.5
1	B	171	TYR	6.4
1	B	83	SER	6.4
1	B	384	ALA	6.4
1	A	85	PHE	6.4
1	B	438	VAL	6.4
1	A	323	TYR	6.4
1	B	312	PHE	6.3
1	B	245	TYR	6.3
1	A	334	GLY	6.3
1	A	246	ALA	6.3
1	A	353	LEU	6.3
1	B	328	CYS	6.3
1	B	126	ILE	6.3
1	B	234	VAL	6.3
1	A	36	TRP	6.3
1	B	162	THR	6.2
1	A	70	TYR	6.2
1	A	173	ALA	6.2
1	A	58	ILE	6.2
1	A	254	ILE	6.2
1	A	275	THR	6.2
1	A	381	TYR	6.2
1	A	398	ILE	6.2
1	B	305	TRP	6.2
1	A	267	TYR	6.2
1	B	94	THR	6.2
1	B	58	ILE	6.2
1	B	363	ILE	6.2
1	A	42	THR	6.1
1	A	190	ILE	6.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	138	ILE	6.1
1	B	137	GLN	6.1
1	A	297	THR	6.1
1	B	267	TYR	6.1
1	B	224	PHE	6.1
1	B	356	ILE	6.1
1	B	250	LEU	6.0
1	B	322	PHE	6.0
1	A	192	ILE	6.0
1	A	363	ILE	6.0
1	B	36	TRP	6.0
1	A	239	MET	6.0
1	A	328	CYS	6.0
1	A	385	TYR	6.0
1	B	379	ASN	6.0
1	A	188	THR	6.0
1	A	139	LEU	5.9
1	B	73	LEU	5.9
1	B	447	LEU	5.9
1	B	416	PRO	5.9
1	A	316	THR	5.9
1	B	152	ASN	5.9
1	A	214	ILE	5.9
1	B	229	ILE	5.9
1	A	262	VAL	5.9
1	B	241	PHE	5.9
1	B	47	GLY	5.9
1	B	192	ILE	5.9
1	B	176	ILE	5.8
1	A	349	VAL	5.8
1	B	159	SER	5.8
1	B	102	PRO	5.8
1	A	422	TYR	5.8
1	B	141	THR	5.8
1	B	344	SER	5.8
1	A	410	THR	5.8
1	A	416	PRO	5.8
1	A	202	TYR	5.8
1	A	362	PHE	5.8
1	B	226	LYS	5.7
1	B	56	ASN	5.7
1	B	139	LEU	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	226	LYS	5.7
1	B	273	PRO	5.7
1	A	445	PHE	5.7
1	A	156	VAL	5.7
1	B	142	VAL	5.7
1	A	115	TRP	5.6
1	A	253	PRO	5.6
1	B	342	LEU	5.6
1	B	180	LYS	5.6
1	B	32	VAL	5.6
1	B	343	ASN	5.6
1	A	403	SER	5.6
1	B	323	TYR	5.6
1	B	272	ILE	5.5
1	A	234	VAL	5.5
1	B	454	THR	5.5
1	A	189	HIS	5.5
1	A	384	ALA	5.5
1	A	337	LEU	5.5
1	A	82	PHE	5.5
1	A	178	ASN	5.5
1	A	370	ILE	5.5
1	B	423	THR	5.5
1	A	233	VAL	5.5
1	B	34	VAL	5.5
1	B	78	ASP	5.5
1	A	378	SER	5.4
1	A	443	PHE	5.4
1	B	74	PHE	5.4
1	B	183	PHE	5.4
1	A	447	LEU	5.4
1	B	220	LEU	5.4
1	B	297	THR	5.4
1	A	171	TYR	5.4
1	B	385	TYR	5.4
1	A	98	ALA	5.4
1	A	84	ILE	5.4
1	A	284	ILE	5.4
1	B	407	ILE	5.4
1	B	461	SER	5.4
1	A	449	PRO	5.4
1	B	332	TYR	5.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	343	ASN	5.4
1	B	324	TRP	5.4
1	B	353	LEU	5.4
1	B	88	ILE	5.4
1	B	99	ASP	5.4
1	A	264	ALA	5.4
1	B	354	TYR	5.3
1	B	77	THR	5.3
1	B	289	VAL	5.3
1	B	396	VAL	5.3
1	B	375	ASN	5.3
1	A	356	ILE	5.3
1	B	395	ILE	5.3
1	B	129	ILE	5.3
1	B	315	ILE	5.3
1	B	98	ALA	5.3
1	B	397	ALA	5.3
1	A	80	ALA	5.3
1	A	86	ARG	5.2
1	B	140	TYR	5.2
1	B	376	PRO	5.2
1	B	337	LEU	5.2
1	B	393	PHE	5.2
1	B	136	ASP	5.2
1	A	448	ALA	5.2
1	A	292	MET	5.2
1	A	143	TRP	5.2
1	A	235	PHE	5.2
1	B	341	ASP	5.2
1	B	57	ASN	5.2
1	A	272	ILE	5.1
1	A	169	ALA	5.1
1	A	401	GLY	5.1
1	A	199	GLU	5.1
1	A	72	LEU	5.1
1	A	399	ASN	5.1
1	A	162	THR	5.0
1	A	268	GLY	5.0
1	B	383	THR	5.0
1	A	289	VAL	5.0
1	B	377	VAL	5.0
1	B	325	TRP	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	455	PHE	5.0
1	A	38	THR	5.0
1	B	147	ALA	5.0
1	A	396	VAL	5.0
1	B	61	LEU	5.0
1	A	245	TYR	5.0
1	A	258	ARG	5.0
1	B	369	ARG	5.0
1	A	458	ASP	5.0
1	B	406	SER	5.0
1	B	145	PRO	5.0
1	A	52	PHE	5.0
1	B	95	TRP	5.0
1	B	390	THR	5.0
1	B	422	TYR	5.0
1	B	350	ALA	5.0
1	A	131	SER	4.9
1	A	73	LEU	4.9
1	A	212	LEU	4.9
1	B	259	VAL	4.9
1	B	355	THR	4.9
1	B	69	ILE	4.9
1	A	257	LYS	4.9
1	A	436	ILE	4.9
1	B	321	TRP	4.9
1	B	446	GLU	4.9
1	B	135	VAL	4.9
1	A	375	ASN	4.8
1	A	183	PHE	4.8
1	A	75	SER	4.8
1	A	347	TYR	4.8
1	A	409	TYR	4.8
1	B	168	TYR	4.8
1	A	126	ILE	4.8
1	A	294	GLY	4.8
1	B	253	PRO	4.8
1	A	111	ASP	4.8
1	A	206	ARG	4.8
1	A	213	ARG	4.8
1	A	96	GLY	4.8
1	B	433	GLY	4.8
1	B	388	PRO	4.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	141	THR	4.7
1	B	338	ILE	4.7
1	A	256	VAL	4.7
1	A	423	THR	4.7
1	B	453	THR	4.7
1	A	218	ASP	4.7
1	A	187	ILE	4.7
1	B	174	GLU	4.7
1	A	140	TYR	4.7
1	A	228	ASN	4.7
1	A	437	THR	4.7
1	A	397	ALA	4.7
1	B	92	GLY	4.7
1	A	37	ASP	4.7
1	A	196	PRO	4.6
1	B	398	ILE	4.6
1	A	444	SER	4.6
1	A	95	TRP	4.6
1	B	359	PHE	4.6
1	A	281	GLY	4.6
1	A	165	TYR	4.6
1	A	382	VAL	4.6
1	B	382	VAL	4.6
1	A	205	CYS	4.6
1	A	134	GLY	4.6
1	B	185	ILE	4.6
1	A	388	PRO	4.6
1	A	266	ASN	4.5
1	A	377	VAL	4.5
1	B	440	ASN	4.5
1	B	30	SER	4.5
1	B	181	SER	4.5
1	A	350	ALA	4.5
1	B	62	GLY	4.5
1	B	404	LYS	4.5
1	B	298	THR	4.5
1	B	215	PHE	4.5
1	B	40	TYR	4.5
1	B	79	GLY	4.5
1	A	78	ASP	4.5
1	B	292	MET	4.5
1	A	148	TRP	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	159	SER	4.4
1	B	333	ASN	4.4
1	A	366	GLY	4.4
1	A	314	THR	4.4
1	B	262	VAL	4.4
1	B	401	GLY	4.4
1	A	383	THR	4.4
1	A	407	ILE	4.4
1	B	113	TRP	4.4
1	A	219	TYR	4.4
1	B	434	SER	4.4
1	A	249	SER	4.3
1	A	197	ASN	4.3
1	B	194	ASN	4.3
1	B	295	ASN	4.3
1	A	411	LEU	4.3
1	A	298	THR	4.3
1	B	127	ARG	4.3
1	B	380	VAL	4.3
1	B	346	THR	4.3
1	A	346	THR	4.2
1	A	400	ASN	4.2
1	B	320	ALA	4.2
1	A	442[B]	SER	4.2
1	A	77	THR	4.2
1	A	163	ASP	4.2
1	A	373	THR	4.2
1	B	85	PHE	4.2
1	B	131	SER	4.2
1	B	76	THR	4.2
1	B	172	LEU	4.2
1	B	319	ASN	4.2
1	B	118	SER	4.2
1	B	42	THR	4.2
1	A	371	GLU	4.2
1	A	128	ALA	4.1
1	B	80	ALA	4.1
1	B	222	PRO	4.1
1	A	119	ASN	4.1
1	B	368	GLN	4.1
1	B	97	ASN	4.1
1	B	198	LEU	4.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	380	VAL	4.1
1	A	454	THR	4.1
1	A	97	ASN	4.1
1	B	169	ALA	4.1
1	A	389	LYS	4.1
1	A	428	GLN	4.1
1	B	279	SER	4.1
1	B	451	SER	4.1
1	B	128	ALA	4.1
1	A	335	GLU	4.1
1	A	340	MET	4.1
1	B	65	LYS	4.1
1	A	223	THR	4.1
1	B	39	THR	4.1
1	A	269	SER	4.0
1	A	217	ARG	4.0
1	A	395	ILE	4.0
1	A	342	LEU	4.0
1	B	72	LEU	4.0
1	B	255	ALA	4.0
1	B	403	SER	4.0
1	A	227	GLU	4.0
1	B	121	ASP	4.0
1	A	313	MET	4.0
1	B	160	LEU	4.0
1	A	440	ASN	4.0
1	A	325	TRP	4.0
1	A	312	PHE	4.0
1	A	392	LYS	4.0
1	A	181	SER	4.0
1	B	75	SER	4.0
1	B	110	GLU	4.0
1	A	35	ASP	4.0
1	B	256	VAL	3.9
1	B	64	THR	3.9
1	A	327	ALA	3.9
1	A	361	ARG	3.9
1	A	220	LEU	3.9
1	A	424	THR	3.9
1	B	117	GLU	3.9
1	B	310	HIS	3.9
1	A	300	ASN	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	275	THR	3.9
1	B	287	THR	3.9
1	A	45	GLY	3.9
1	B	93	GLY	3.9
1	B	365	PRO	3.9
1	A	136	ASP	3.9
1	A	265	HIS	3.9
1	A	114	ASP	3.9
1	B	426	SER	3.9
1	B	442[A]	SER	3.9
1	B	358	GLN	3.9
1	A	103	ASN	3.9
1	B	125	MET	3.8
1	B	248	ASN	3.8
1	A	161	ARG	3.8
1	A	376	PRO	3.8
1	B	228	ASN	3.8
1	A	276	THR	3.8
1	B	425	SER	3.8
1	B	124	PRO	3.8
1	B	33	THR	3.8
1	B	316	THR	3.8
1	A	47	GLY	3.8
1	A	191	GLY	3.8
1	B	400	ASN	3.8
1	B	448	ALA	3.7
1	A	102	PRO	3.7
1	A	194	ASN	3.7
1	A	255	ALA	3.7
1	A	286	MET	3.7
1	B	37	ASP	3.7
1	A	248	ASN	3.7
1	B	68	GLU	3.7
1	B	107	GLN	3.7
1	A	109	ALA	3.7
1	B	173	ALA	3.7
1	B	231	ALA	3.7
1	A	251	ASN	3.7
1	B	300	ASN	3.7
1	B	60	ARG	3.7
1	B	221	VAL	3.7
1	A	151	THR	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	277	THR	3.7
1	B	308	GLU	3.7
1	A	260	ASP	3.7
1	B	203	SER	3.7
1	A	112	VAL	3.6
1	A	116	ASN	3.6
1	A	179	TYR	3.6
1	A	332	TYR	3.6
1	A	108	PRO	3.6
1	A	320	ALA	3.6
1	A	345	LYS	3.6
1	B	266	ASN	3.6
1	B	217	ARG	3.6
1	B	296	ASP	3.6
1	A	368	GLN	3.6
1	B	374	LYS	3.6
1	A	434	SER	3.6
1	B	269	SER	3.6
1	B	439	ASN	3.6
1	B	364	ARG	3.6
1	B	286	MET	3.6
1	A	39	THR	3.6
1	A	336	GLY	3.6
1	B	331	THR	3.6
1	A	71	ASP	3.6
1	A	182	LYS	3.6
1	A	372	ALA	3.6
1	B	182	LYS	3.6
1	A	79	GLY	3.5
1	B	177	LYS	3.5
1	A	236	ALA	3.5
1	A	421	PRO	3.5
1	A	203	SER	3.5
1	B	71	ASP	3.5
1	A	63[A]	GLU	3.5
1	A	124	PRO	3.5
1	B	293	ASN	3.5
1	B	449	PRO	3.5
1	B	450	ASN	3.5
1	A	240	SER	3.5
1	B	114	ASP	3.5
1	A	175	HIS	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	81	GLY	3.5
1	B	153	GLY	3.5
1	A	117	GLU	3.5
1	B	55	SER	3.5
1	B	276	THR	3.5
1	A	209	PRO	3.5
1	B	67	ASN	3.4
1	A	355	THR	3.4
1	B	301	ASP	3.4
1	B	302	GLY	3.4
1	B	122	GLN	3.4
1	B	186	GLU	3.4
1	A	360	SER	3.4
1	A	291	ASP	3.4
1	A	357	GLY	3.4
1	B	200	THR	3.4
1	A	93	GLY	3.4
1	B	336	GLY	3.4
1	B	373	THR	3.4
1	A	83	SER	3.4
1	B	225	ASP	3.4
1	A	201	SER	3.4
1	A	290	SER	3.4
1	B	444	SER	3.4
1	B	413	GLY	3.3
1	A	147	ALA	3.3
1	A	369	ARG	3.3
1	B	361	ARG	3.3
1	A	88	ILE	3.3
1	B	408	THR	3.3
1	B	265	HIS	3.3
1	B	405	GLN	3.3
1	B	209	PRO	3.3
1	B	195	GLU	3.3
1	A	65	LYS	3.3
1	A	216	MET	3.3
1	B	53	HIS	3.3
1	B	193	GLN	3.3
1	B	457	GLY	3.3
1	A	208	SER	3.3
1	A	426	SER	3.3
1	B	304	ARG	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	51	ALA	3.3
1	B	349	VAL	3.3
1	A	56	ASN	3.3
1	A	310	HIS	3.3
1	B	257	LYS	3.3
1	B	458	ASP	3.3
1	A	295	ASN	3.3
1	B	372	ALA	3.3
1	B	313	MET	3.3
1	A	91	ASP	3.2
1	A	365	PRO	3.2
1	B	238	ASN	3.2
1	B	412	LYS	3.2
1	A	306	ALA	3.2
1	B	339	GLN	3.2
1	A	177	LYS	3.2
1	A	277	THR	3.2
1	B	258	ARG	3.2
1	A	441	SER	3.2
1	B	240	SER	3.2
1	B	263	GLY	3.2
1	A	204	SER	3.2
1	A	425	SER	3.2
1	A	62	GLY	3.2
1	A	174	GLU	3.2
1	B	239	MET	3.2
1	B	264	ALA	3.2
1	B	196	PRO	3.1
1	A	333	ASN	3.1
1	A	420	THR	3.1
1	A	404	LYS	3.1
1	B	164	LYS	3.1
1	A	406	SER	3.1
1	A	94	THR	3.1
1	B	314	THR	3.1
1	B	348	LYS	3.1
1	B	144	SER	3.1
1	B	419	VAL	3.1
1	B	86	ARG	3.1
1	A	167	ALA	3.1
1	A	302	GLY	3.1
1	A	57	ASN	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	237	GLU	3.1
1	A	432	LYS	3.1
1	B	134	GLY	3.0
1	B	334	GLY	3.0
1	A	137	GLN	3.0
1	A	152	ASN	3.0
1	B	340	MET	3.0
1	B	105	THR	3.0
1	B	249	SER	3.0
1	B	399	ASN	3.0
1	A	200	THR	3.0
1	A	318	GLY	3.0
1	B	103	ASN	3.0
1	A	180	LYS	3.0
1	A	270	SER	3.0
1	B	45	GLY	3.0
1	B	204	SER	3.0
1	B	278	LYS	3.0
1	A	358	GLN	3.0
1	A	186	GLU	2.9
1	B	237	GLU	2.9
1	A	307	LYS	2.9
1	A	374	LYS	2.9
1	B	163	ASP	2.9
1	A	244	GLN	2.9
1	B	244	GLN	2.9
1	B	394	ALA	2.9
1	A	90	GLY	2.9
1	B	184	GLY	2.9
1	B	421	PRO	2.9
1	B	120	ASP	2.9
1	A	106	MET	2.8
1	B	366	GLY	2.8
1	A	44	ASP	2.8
1	A	193	GLN	2.8
1	A	417	ALA	2.8
1	B	387	ASP	2.8
1	B	158	GLY	2.8
1	A	304	ARG	2.8
1	B	211	GLU	2.8
1	B	91	ASP	2.8
1	A	184	GLY	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	197	ASN	2.8
1	A	146	PRO	2.8
1	B	170	THR	2.8
1	B	459	THR	2.8
1	A	41	GLN	2.8
1	B	391	GLY	2.8
1	B	242	ASN	2.8
1	B	345	LYS	2.8
1	A	405	GLN	2.8
1	A	132	LYS	2.7
1	A	230	THR	2.7
1	B	410	THR	2.7
1	B	81	GLY	2.7
1	B	167	ALA	2.7
1	A	232	LYS	2.7
1	A	351	LYS	2.7
1	B	104	LYS	2.7
1	A	158	GLY	2.7
1	A	301	ASP	2.7
1	A	387	ASP	2.7
1	A	451	SER	2.7
1	B	157	GLY	2.7
1	B	357	GLY	2.7
1	B	106	MET	2.7
1	B	429	ASN	2.7
1	B	205	CYS	2.7
1	A	130	GLN	2.7
1	B	307	LYS	2.6
1	A	164	LYS	2.6
1	A	242	ASN	2.6
1	A	280	LYS	2.6
1	B	216	MET	2.6
1	A	59	ALA	2.6
1	A	450	ASN	2.6
1	A	427	THR	2.6
1	B	420	THR	2.6
1	B	291	ASP	2.6
1	B	178	ASN	2.6
1	B	288	GLU	2.6
1	B	330	LYS	2.6
1	A	287	THR	2.6
1	B	326	GLY	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	100	ASP	2.6
1	B	49	SER	2.6
1	B	166	GLN	2.6
1	B	243	GLU	2.6
1	A	429	ASN	2.6
1	A	157	GLY	2.5
1	A	446	GLU	2.5
1	B	280	LYS	2.5
1	A	238	ASN	2.5
1	A	379	ASN	2.5
1	A	166	GLN	2.5
1	A	341	ASP	2.5
1	B	66	GLN	2.5
1	A	211	GLU	2.5
1	B	35	ASP	2.5
1	B	199	GLU	2.5
1	B	132	LYS	2.5
1	A	99	ASP	2.5
1	A	296	ASP	2.5
1	A	87	SER	2.5
1	A	415	SER	2.5
1	B	149	MET	2.5
1	B	281	GLY	2.5
1	B	432	LYS	2.5
1	A	435	ASP	2.5
1	A	319	ASN	2.4
1	B	318	GLY	2.4
1	A	278	LYS	2.4
1	B	100	ASP	2.4
1	B	360	SER	2.4
1	A	273	PRO	2.4
1	B	150	LYS	2.4
1	B	208	SER	2.4
1	A	243	GLU	2.3
1	A	433	GLY	2.3
1	B	227	GLU	2.3
1	A	49	SER	2.3
1	A	282	LYS	2.3
1	B	155	VAL	2.3
1	B	191	GLY	2.3
1	A	154	SER	2.3
1	B	418	SER	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	453	THR	2.3
1	B	260	ASP	2.3
1	A	386	LYS	2.3
1	B	282	LYS	2.3
1	A	53	HIS	2.3
1	B	210	GLU	2.3
1	B	232	LYS	2.3
1	A	54	GLN	2.3
1	A	67	ASN	2.3
1	A	101	GLY	2.3
1	B	44	ASP	2.2
1	A	125	MET	2.2
1	B	50	GLU	2.2
1	A	311	ASP	2.2
1	B	218	ASP	2.2
1	A	457	GLY	2.2
1	B	283	GLY	2.2
1	A	431	GLU	2.2
1	B	435	ASP	2.2
1	A	144	SER	2.2
1	A	413	GLY	2.2
1	A	418	SER	2.2
1	B	351	LYS	2.2
1	B	189	HIS	2.2
1	B	352	ARG	2.2
1	B	111	ASP	2.2
1	B	268	GLY	2.2
1	A	348	LYS	2.2
1	A	288	GLU	2.1
1	B	335	GLU	2.1
1	B	90	GLY	2.1
1	A	127	ARG	2.1
1	B	311	ASP	2.1
1	A	210	GLU	2.1
1	B	130	GLN	2.1
1	B	206	ARG	2.1
1	A	120	ASP	2.1
1	B	96	GLY	2.1
1	B	294	GLY	2.1
1	A	339	GLN	2.0
1	A	107	GLN	2.0
1	A	122	GLN	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	101	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	A	517	4/4	0.30	0.31	21,21,22,22	0
3	ACT	A	516	4/4	0.33	0.29	17,18,20,21	0
2	CL	A	511	1/1	0.37	0.49	33,33,33,33	0
2	CL	A	506	1/1	0.39	0.45	45,45,45,45	0
2	CL	A	501	1/1	0.46	0.29	39,39,39,39	0
2	CL	A	509	1/1	0.48	0.38	68,68,68,68	0
2	CL	A	502	1/1	0.49	0.15	31,31,31,31	0
2	CL	A	513	1/1	0.49	0.22	49,49,49,49	0
2	CL	A	503	1/1	0.51	0.20	52,52,52,52	0
3	ACT	B	509	4/4	0.61	0.31	24,24,26,27	0
2	CL	A	510	1/1	0.64	0.20	50,50,50,50	0
2	CL	B	507	1/1	0.66	0.54	79,79,79,79	0
2	CL	B	506	1/1	0.66	0.20	27,27,27,27	0
2	CL	A	507	1/1	0.67	0.33	23,23,23,23	0
2	CL	B	501	1/1	0.72	0.25	33,33,33,33	0
2	CL	B	505	1/1	0.73	0.25	38,38,38,38	0
2	CL	A	505	1/1	0.73	0.11	29,29,29,29	0
2	CL	A	514	1/1	0.74	0.21	45,45,45,45	0
2	CL	B	502	1/1	0.74	0.10	23,23,23,23	0
2	CL	A	512	1/1	0.75	0.22	40,40,40,40	0
2	CL	A	504	1/1	0.76	0.46	48,48,48,48	0
2	CL	A	515	1/1	0.78	0.21	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	A	508	1/1	0.81	0.17	22,22,22,22	0
2	CL	B	504	1/1	0.82	0.24	39,39,39,39	0
2	CL	B	508	1/1	0.88	0.16	45,45,45,45	0
2	CL	B	503	1/1	0.91	0.06	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.